FASTMath Integrated Technologies

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Integration of structured and unstructured mesh technologies with advanced solution methods to impact complex multiphysics applications

Albany – Trilinos/PUMI Integration

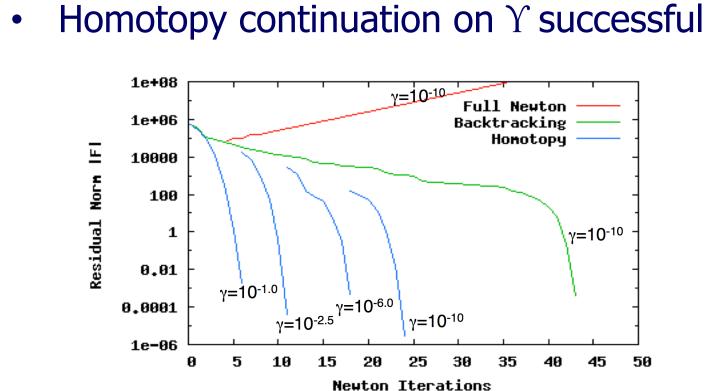Finite element application development environment
- Albany is based on *AgileComponents* strategy
- Extensive set of physics components, residual pattern simplifies adding new models
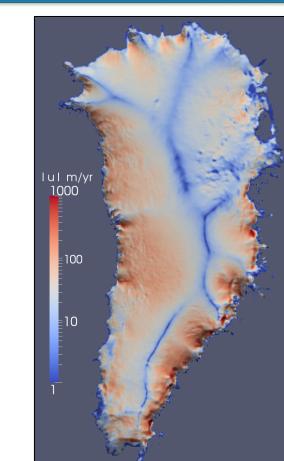- TBGP-Sacado: derivatives automatically formed for Jacobian, SA, and UQ
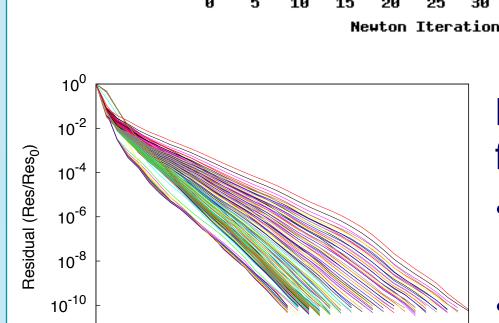

ML/NOX/LOCA Solution Components

Ice Sheet modeled by nonlinear Stokes equation
- Initial solve is fragile: full Newton fails
- Homotopy continuation on Υ successful

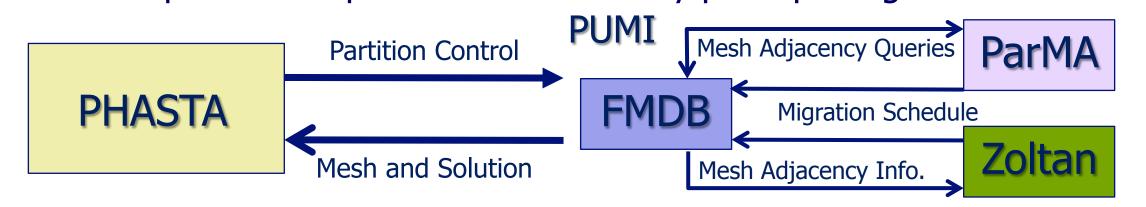Greenland Ice Sheet Surface Velocities
(constant friction model)

ML preconditioned NOX solve of nuclear fuel hydride reorientation problem
- LOCA continuation-driven loading generates convergence trajectories
- Albany supplies rigid body modes to ML to accelerate convergence

PHASTA - PUMI: Partitioning to 3 Million Parts

Suite of partitioning tools integrated into PHASTA pre-processor to partition massively unstructured meshes.
- Zoltan graph/hyper-graph and geometric methods
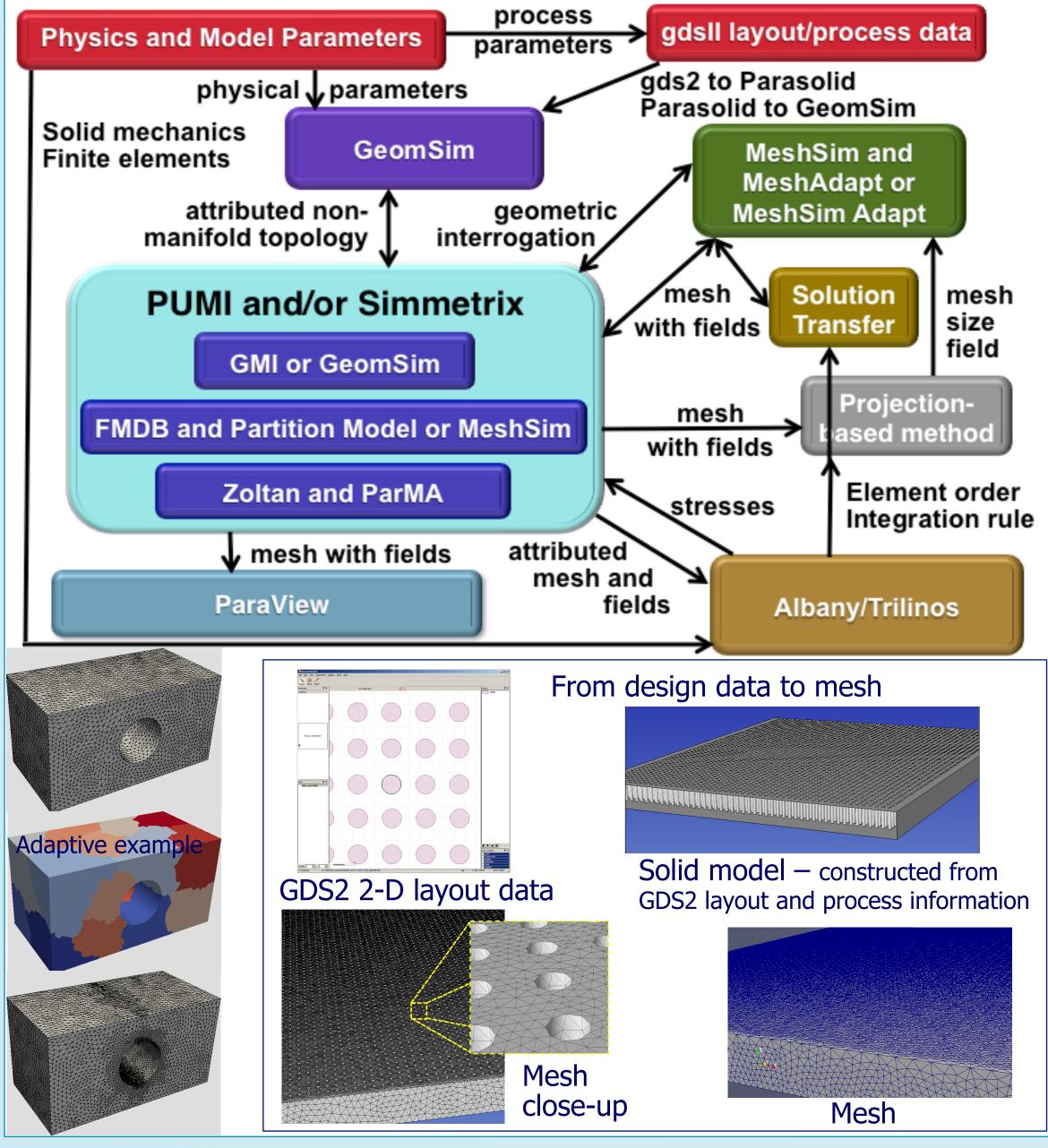- ParMA partition improvement and heavy part splitting

Bringing Adaptivity to Albany

Component-based approach to automated adaptive simulations
- Albany – Trilinos-based demonstration FE based analysis engine
- PUMI/MeshAdapt – parallel unstructured mesh adaptivity
- All steps can execute in parallel including initial mesh generation
- In-memory API's used to integrate adaptive loop components

Simulations being developed
- Mechanics of integrated circuits starting from design data
- Weld failures
- Shape optimization

Components to address the mechanics of integrated circuit application (emphasis on the parallel unstructured mesh core)

From design data to mesh

GDS2 2-D layout data

Solid model – constructed from GDS2 layout and process information

Adaptive example
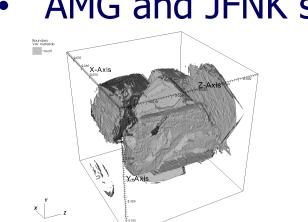
Mesh close-up

Mesh

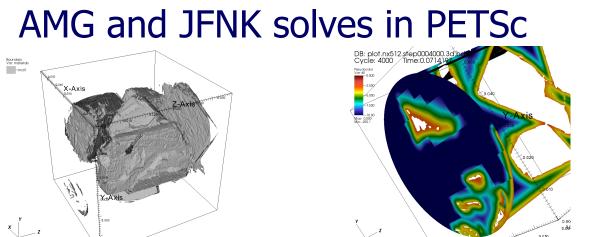## High Resolution AMR - BISICLES/EBAMRINS
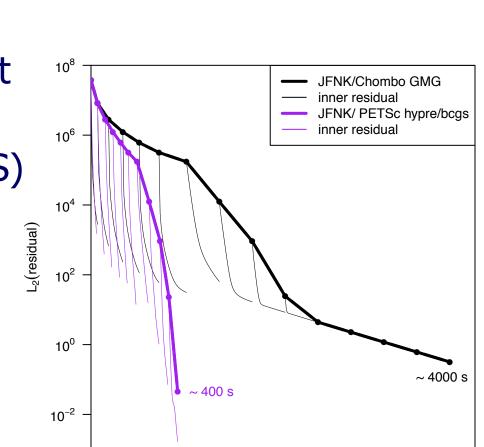
Chombo-based AMR for land ice sheets
- Highly nonlinear, coupled elliptic system
- large jumps in material coefficients
- JFNK/Chombo GMG, JFNK/PETSc GAMG – hypre/bcgs
- In experiments, GAMG is significantly faster and more robust than GMG on this problem

Embedded boundary AMR (EBAMRINS)
- Linearize set of patches on a level
- Create explicit matrix of stencil
- AMG and JFNK solves in PETSc

(right) Computed ice velocity for Antarctica; (left) meshing and grounding line location for the Pine Island Glacier.
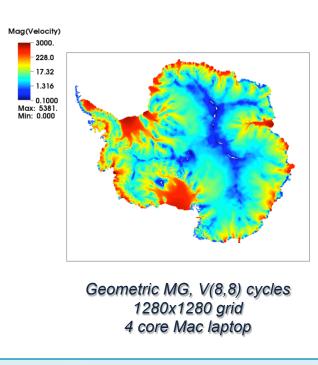
Application List

- BISICLES Ice Sheet Modeling (Chombo/AMR)
- PISCEES Ice Sheet Modeling (Albany)
- Porous media flow with complex boundaries (Chombo/AMR)
- Nuclear reactor multiphase flow, fuel response (PHASTA, Albany)
- Mechanics of integrated circuits (Albany)

Geometric MG, V(8,8) cycles
1280x1280 grid
4 core Mac laptop

Future Plans

Chombo PETSc Integration
- Fully deploy and support AMR - JFNK - AMG solver in BISICLES
- Add AMR - AMG support for EBAMRINS
- Add interface to COGENT (LLNL) Vlasov code

Albany/PUMI Integration
- Develop general solution transfer capabilities
- Build error-based adaptation classes to couple with with physics evaluation framework

More Information: http://www.fastmath-scidac.org or contact Lori Diachin, LLNL, diachin2@llnl.gov, 925-422-7130